



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 28, 2026 – 07:35 AM UTC

PDB ID : 7T1W / pdb_00007t1w
Title : Crystal structure of human Fab A194-01 in complex with its synthetic tetrasaccharide Ara4 epitope (BSI110886)
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2021-12-02
Resolution : 2.45 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

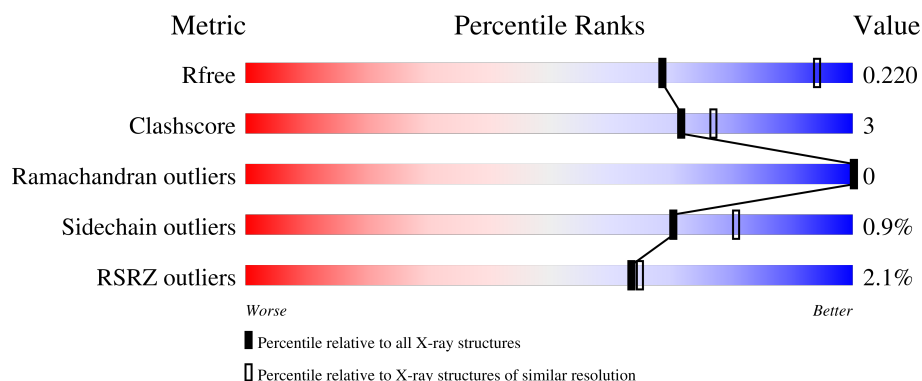
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	H	228	
1	H2	228	
1	H3	228	
1	H4	228	
1	H5	228	

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Mol	Chain	Length	Quality of chain
2	L	213	92% 8%
2	L2	213	96%
2	L3	213	2% 91% 9%
2	L4	213	93% 7%
2	L5	213	% 95% 5%
3	A	4	100%
3	B	4	25% 75%
3	C	4	50% 50%
3	D	4	75% 25%
3	E	4	25% 75%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17570 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Fab A194-01 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	216	Total	C	N	O	S	0	3	0
			1648	1042	280	319	7			
1	H2	217	Total	C	N	O	S	0	2	0
			1631	1031	272	321	7			
1	H3	215	Total	C	N	O	S	0	0	0
			1571	991	263	310	7			
1	H4	217	Total	C	N	O	S	0	1	0
			1640	1039	276	318	7			
1	H5	217	Total	C	N	O	S	0	0	0
			1594	1007	265	315	7			

- Molecule 2 is a protein called Fab A194-01 light chain.

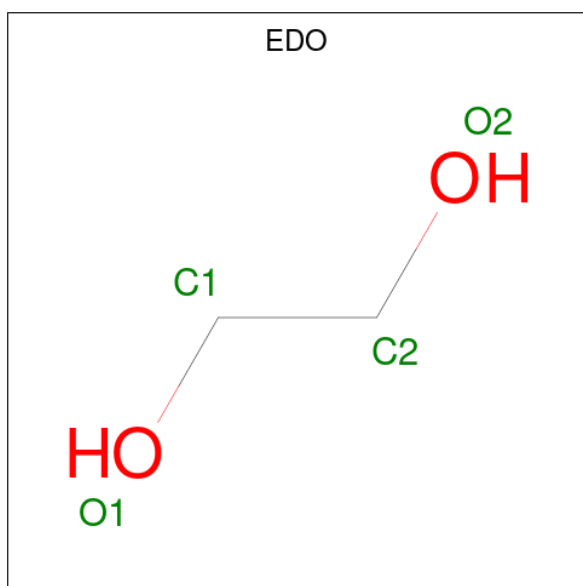
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	213	Total	C	N	O	S	0	1	0
			1624	1014	281	324	5			
2	L2	213	Total	C	N	O	S	0	2	0
			1634	1024	281	324	5			
2	L3	213	Total	C	N	O	S	0	2	0
			1609	1004	281	319	5			
2	L4	212	Total	C	N	O	S	0	1	0
			1615	1008	279	323	5			
2	L5	213	Total	C	N	O	S	0	0	0
			1602	1000	277	320	5			

- Molecule 3 is an oligosaccharide called beta-D-arabinofuranose-(1-2)-alpha-D-arabinofuranose-(1-5)-alpha-D-arabinofuranose-(1-5)-alpha-D-arabinofuranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	A	4	Total	C	O	0	0	0
			37	20	17			
3	B	4	Total	C	O	0	0	0
			37	20	17			
3	C	4	Total	C	O	0	0	0
			37	20	17			
3	D	4	Total	C	O	0	1	0
			46	25	21			
3	E	4	Total	C	O	0	0	0
			37	20	17			

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



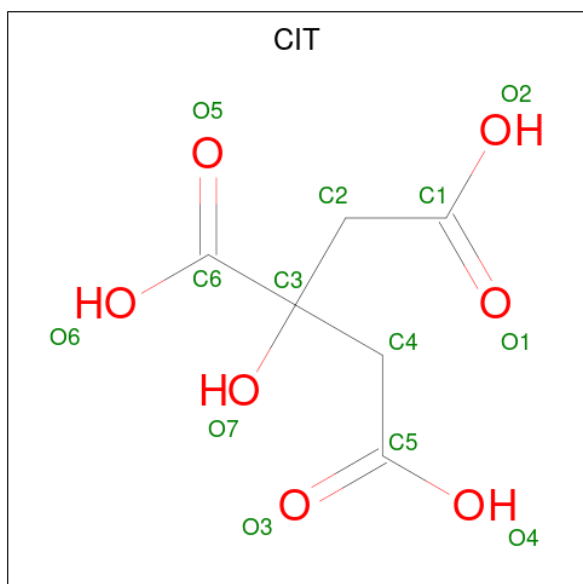
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	1
			8	4	4		
4	L	1	Total	C	O	0	0
			4	2	2		
4	H2	1	Total	C	O	0	0
			4	2	2		
4	H2	1	Total	C	O	0	0
			4	2	2		
4	H3	1	Total	C	O	0	0
			4	2	2		
4	H3	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	L3	1	Total	C	O	0	0
			4	2	2		
4	L3	1	Total	C	O	0	0
			4	2	2		
4	H4	1	Total	C	O	0	0
			4	2	2		
4	H4	1	Total	C	O	0	0
			4	2	2		
4	L4	1	Total	C	O	0	0
			4	2	2		
4	H5	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L4	1	Total	C	O	0	0
			13	6	7		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	141	Total	O	0	2
			143	143		
6	L	167	Total	O	0	1
			168	168		

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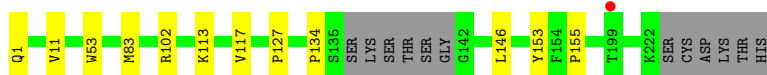
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H2	94	Total 94	O 94	0	0
6	L2	110	Total 110	O 110	0	0
6	H3	59	Total 59	O 59	0	0
6	L3	98	Total 98	O 98	0	0
6	H4	152	Total 156	O 156	0	4
6	L4	111	Total 111	O 111	0	0
6	H5	107	Total 107	O 107	0	0
6	L5	92	Total 93	O 93	0	1

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

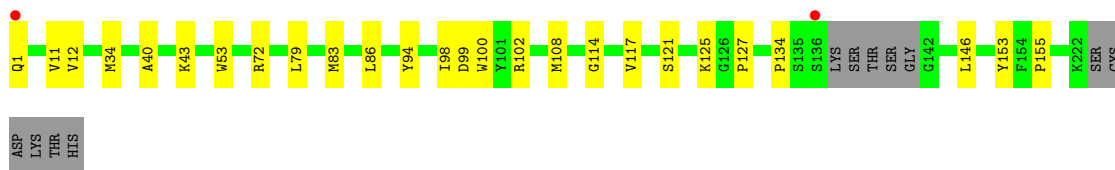
- Molecule 1: Fab A194-01 heavy chain

Chain H: 



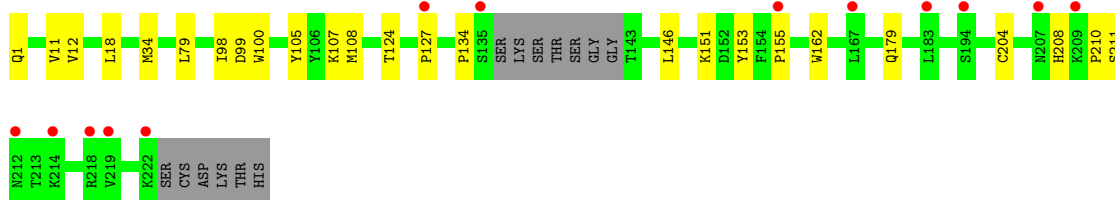
- Molecule 1: Fab A194-01 heavy chain

Chain H2: 



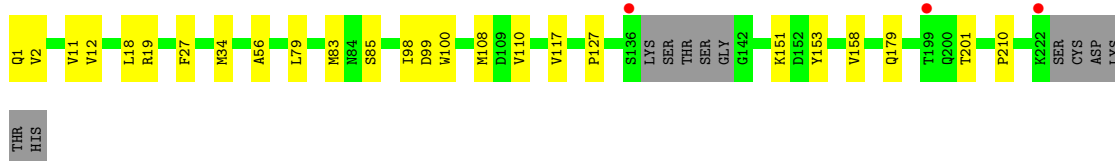
- Molecule 1: Fab A194-01 heavy chain

Chain H3: 

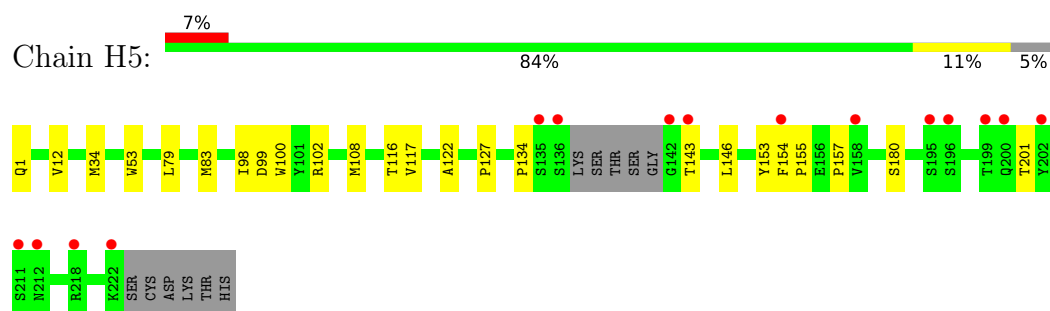


- Molecule 1: Fab A194-01 heavy chain

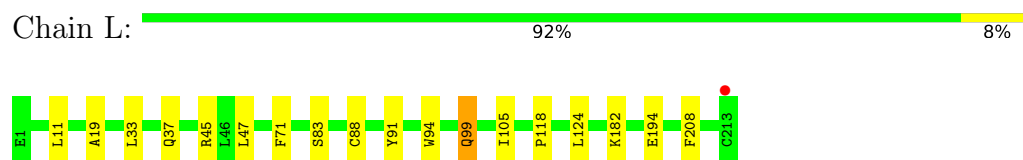
Chain H4: 



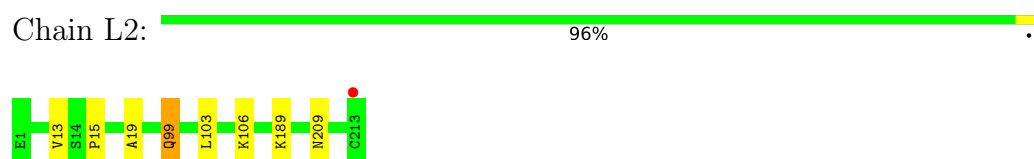
- Molecule 1: Fab A194-01 heavy chain



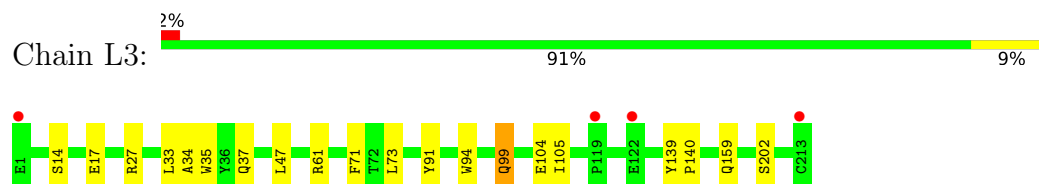
- Molecule 2: Fab A194-01 light chain



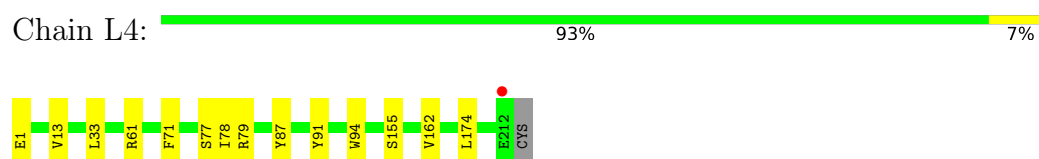
- Molecule 2: Fab A194-01 light chain



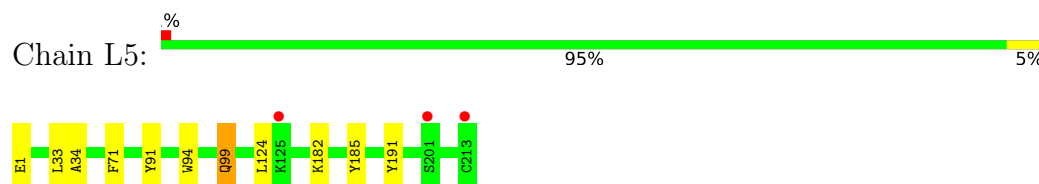
- Molecule 2: Fab A194-01 light chain



- Molecule 2: Fab A194-01 light chain



- Molecule 2: Fab A194-01 light chain



- Molecule 3: beta-D-arabinofuranose-(1-2)-alpha-D-arabinofuranose-(1-5)-alpha-D-arabinofuranose-(1-5)-alpha-D-arabinofuranose

Chain A:  100%

EXY1
EXY2
EXY3
EXY4

- Molecule 3: beta-D-arabinofuranose-(1-2)-alpha-D-arabinofuranose-(1-5)-alpha-D-arabinofuranose-(1-5)-alpha-D-arabinofuranose

Chain B:  25% 75%

EXY1
EXY2
EXY3
EXY4

- Molecule 3: beta-D-arabinofuranose-(1-2)-alpha-D-arabinofuranose-(1-5)-alpha-D-arabinofuranose-(1-5)-alpha-D-arabinofuranose

Chain C:  50% 50%

EXY1
EXY2
EXY3
EXY4

- Molecule 3: beta-D-arabinofuranose-(1-2)-alpha-D-arabinofuranose-(1-5)-alpha-D-arabinofuranose-(1-5)-alpha-D-arabinofuranose

Chain D:  75% 25%

EXY1
EXY2
EXY3
EXY4

- Molecule 3: beta-D-arabinofuranose-(1-2)-alpha-D-arabinofuranose-(1-5)-alpha-D-arabinofuranose-(1-5)-alpha-D-arabinofuranose

Chain E:  25% 75%

EXY1
EXY2
EXY3
EXY4

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.62Å 149.01Å 114.53Å 90.00° 99.51° 90.00°	Depositor
Resolution (Å)	45.47 – 2.45 45.47 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.0 (45.47-2.45) 99.0 (45.47-2.45)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.18rc1 3776	Depositor
R, R_{free}	0.168 , 0.218 0.171 , 0.220	Depositor DCC
R_{free} test set	1983 reflections (1.91%)	wwPDB-VP
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17570	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BXY, BXX, CIT, EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	H	0.21	0/1694	0.47	0/2306
1	H2	0.19	0/1677	0.46	0/2288
1	H3	0.19	0/1611	0.44	0/2204
1	H4	0.21	0/1683	0.47	0/2292
1	H5	0.21	0/1634	0.47	0/2234
2	L	0.21	0/1663	0.47	0/2263
2	L2	0.19	0/1676	0.43	0/2278
2	L3	0.20	0/1651	0.44	0/2250
2	L4	0.21	0/1654	0.44	0/2252
2	L5	0.19	0/1638	0.42	0/2232
All	All	0.20	0/16581	0.45	0/22599

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1648	0	1601	6	0
1	H2	1631	0	1560	15	0
1	H3	1571	0	1448	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H4	1640	0	1594	14	0
1	H5	1594	0	1491	13	0
2	L	1624	0	1549	11	0
2	L2	1634	0	1580	5	0
2	L3	1609	0	1517	12	0
2	L4	1615	0	1536	8	0
2	L5	1602	0	1510	7	0
3	A	37	0	31	0	0
3	B	37	0	31	0	0
3	C	37	0	31	0	0
3	D	46	0	40	2	0
3	E	37	0	31	0	0
4	H	12	0	18	0	0
4	H2	8	0	12	1	0
4	H3	8	0	12	0	0
4	H4	8	0	12	1	0
4	H5	4	0	6	0	0
4	L	4	0	6	0	0
4	L3	8	0	12	1	0
4	L4	4	0	6	0	0
5	L4	13	0	5	1	0
6	H	143	0	0	1	1
6	H2	94	0	0	2	0
6	H3	59	0	0	1	0
6	H4	156	0	0	2	0
6	H5	107	0	0	2	0
6	L	168	0	0	1	0
6	L2	110	0	0	0	0
6	L3	98	0	0	2	1
6	L4	111	0	0	0	0
6	L5	93	0	0	1	0
All	All	17570	0	15639	105	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 105 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H5:1:GLN:N	6:H5:601:HOH:O	2.08	0.84
1:H2:72:ARG:HG3	4:H2:502:EDO:H11	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H3:11:VAL:HG22	1:H3:155:PRO:HG3	1.71	0.71
1:H:134:PRO:HG3	1:H:146:LEU:HB3	1.71	0.71
1:H5:134:PRO:HG3	1:H5:146:LEU:HB3	1.74	0.70

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:698:HOH:O	6:L3:480:HOH:O[2_454]	2.16	0.04

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	215/228 (94%)	210 (98%)	5 (2%)	0	100	100
1	H2	215/228 (94%)	209 (97%)	6 (3%)	0	100	100
1	H3	211/228 (92%)	207 (98%)	4 (2%)	0	100	100
1	H4	214/228 (94%)	210 (98%)	4 (2%)	0	100	100
1	H5	213/228 (93%)	207 (97%)	6 (3%)	0	100	100
2	L	212/213 (100%)	207 (98%)	5 (2%)	0	100	100
2	L2	213/213 (100%)	208 (98%)	5 (2%)	0	100	100
2	L3	213/213 (100%)	208 (98%)	5 (2%)	0	100	100
2	L4	211/213 (99%)	206 (98%)	5 (2%)	0	100	100
2	L5	211/213 (99%)	207 (98%)	4 (2%)	0	100	100
All	All	2128/2205 (96%)	2079 (98%)	49 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	182/192 (95%)	181 (100%)	1 (0%)	81	87
1	H2	179/192 (93%)	179 (100%)	0	100	100
1	H3	164/192 (85%)	164 (100%)	0	100	100
1	H4	181/192 (94%)	178 (98%)	3 (2%)	53	67
1	H5	170/192 (88%)	166 (98%)	4 (2%)	43	58
2	L	177/183 (97%)	176 (99%)	1 (1%)	78	86
2	L2	180/183 (98%)	179 (99%)	1 (1%)	78	86
2	L3	172/183 (94%)	170 (99%)	2 (1%)	63	74
2	L4	176/183 (96%)	174 (99%)	2 (1%)	65	76
2	L5	172/183 (94%)	170 (99%)	2 (1%)	63	74
All	All	1753/1875 (94%)	1737 (99%)	16 (1%)	70	81

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L5	1	GLU
1	H5	201	THR
2	L4	1	GLU
1	H5	180	SER
1	H4	201	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	H4	82	GLN
1	H4	84	ASN
2	L5	188	HIS
2	L5	137	ASN
2	L5	146	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

21 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BXY	A	1	3	10,10,10	0.72	0	13,14,14	1.32	2 (15%)
3	BXY	A	2	3	9,9,10	0.61	0	11,12,14	1.02	1 (9%)
3	BXY	A	3	3	9,9,10	0.98	1 (11%)	11,12,14	1.95	2 (18%)
3	BXX	A	4	3	9,9,10	0.52	0	11,12,14	1.16	1 (9%)
3	BXY	B	1	3	10,10,10	0.75	0	13,14,14	1.45	2 (15%)
3	BXY	B	2	3	9,9,10	0.66	0	11,12,14	0.97	1 (9%)
3	BXY	B	3	3	9,9,10	0.97	1 (11%)	11,12,14	2.17	4 (36%)
3	BXX	B	4	3	9,9,10	0.47	0	11,12,14	0.94	0
3	BXY	C	1	3	10,10,10	0.71	0	13,14,14	3.10	3 (23%)
3	BXY	C	2	3	9,9,10	0.66	0	11,12,14	0.85	0
3	BXY	C	3	3	9,9,10	1.01	1 (11%)	11,12,14	1.93	3 (27%)
3	BXX	C	4	3	9,9,10	0.45	0	11,12,14	0.95	0
3	BXY	D	1[A]	-	10,10,10	0.66	0	13,14,14	1.96	5 (38%)
3	BXY	D	1[B]	-	10,10,10	0.66	0	13,14,14	1.53	4 (30%)
3	BXY	D	2	3	9,9,10	0.66	0	11,12,14	0.89	0
3	BXY	D	3	3	9,9,10	1.02	1 (11%)	11,12,14	1.87	3 (27%)
3	BXX	D	4	3	9,9,10	0.57	0	11,12,14	1.13	1 (9%)
3	BXY	E	1	3	10,10,10	0.68	0	13,14,14	1.60	4 (30%)
3	BXY	E	2	3	9,9,10	0.73	0	11,12,14	1.21	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BXY	E	3	3	9,9,10	0.99	1 (11%)	11,12,14	1.85	2 (18%)
3	BXX	E	4	3	9,9,10	0.50	0	11,12,14	0.96	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BXY	A	1	3	-	2/2/18/18	0/1/1/1
3	BXY	A	2	3	-	0/2/15/18	0/1/1/1
3	BXY	A	3	3	-	2/2/15/18	0/1/1/1
3	BXX	A	4	3	-	0/2/15/18	0/1/1/1
3	BXY	B	1	3	-	2/2/18/18	0/1/1/1
3	BXY	B	2	3	-	0/2/15/18	0/1/1/1
3	BXY	B	3	3	-	0/2/15/18	0/1/1/1
3	BXX	B	4	3	-	0/2/15/18	0/1/1/1
3	BXY	C	1	3	-	0/2/18/18	0/1/1/1
3	BXY	C	2	3	-	0/2/15/18	0/1/1/1
3	BXY	C	3	3	-	0/2/15/18	0/1/1/1
3	BXX	C	4	3	-	0/2/15/18	0/1/1/1
3	BXY	D	1[A]	-	-	2/2/18/18	0/1/1/1
3	BXY	D	1[B]	-	-	2/2/18/18	0/1/1/1
3	BXY	D	2	3	-	0/2/15/18	0/1/1/1
3	BXY	D	3	3	-	1/2/15/18	0/1/1/1
3	BXX	D	4	3	-	0/2/15/18	0/1/1/1
3	BXY	E	1	3	-	0/2/18/18	0/1/1/1
3	BXY	E	2	3	-	0/2/15/18	0/1/1/1
3	BXY	E	3	3	-	0/2/15/18	0/1/1/1
3	BXX	E	4	3	-	0/2/15/18	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	3	BXY	O2-C2	-2.55	1.38	1.43
3	C	3	BXY	O2-C2	-2.54	1.38	1.43
3	D	3	BXY	O2-C2	-2.53	1.38	1.43
3	A	3	BXY	O2-C2	-2.53	1.38	1.43
3	B	3	BXY	O2-C2	-2.48	1.38	1.43

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	BXY	O5-C5-C4	10.12	145.78	111.33
3	A	3	BXY	O2-C2-C1	-4.76	96.07	110.89
3	D	1[A]	BXY	O5-C5-C4	-4.54	95.86	111.33
3	E	3	BXY	O2-C2-C1	-4.49	96.89	110.89
3	C	3	BXY	O2-C2-C1	-4.42	97.14	110.89

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

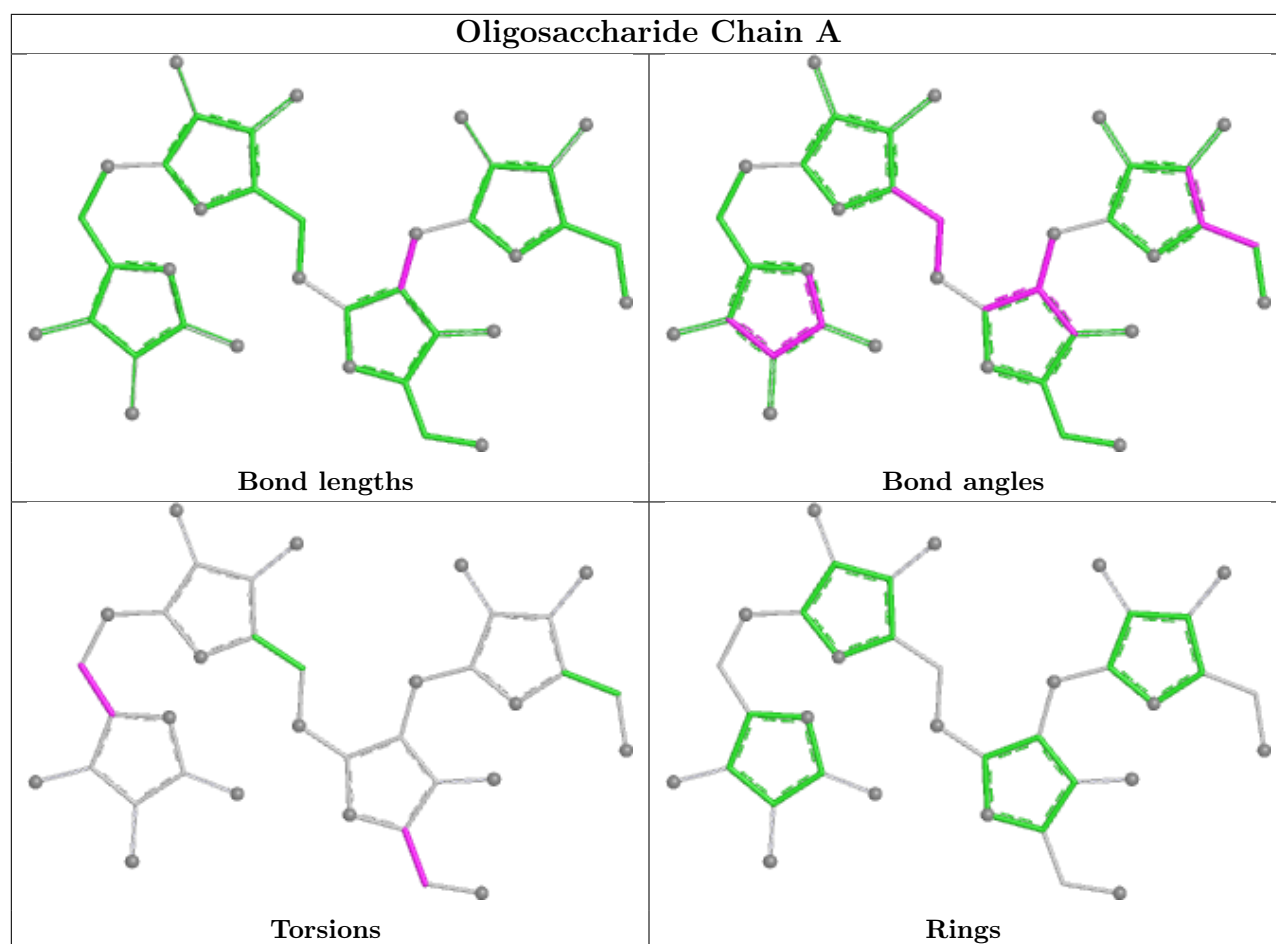
Mol	Chain	Res	Type	Atoms
3	B	1	BXY	O4-C4-C5-O5
3	A	1	BXY	O4-C4-C5-O5
3	A	1	BXY	C3-C4-C5-O5
3	B	1	BXY	C3-C4-C5-O5
3	D	1[B]	BXY	C3-C4-C5-O5

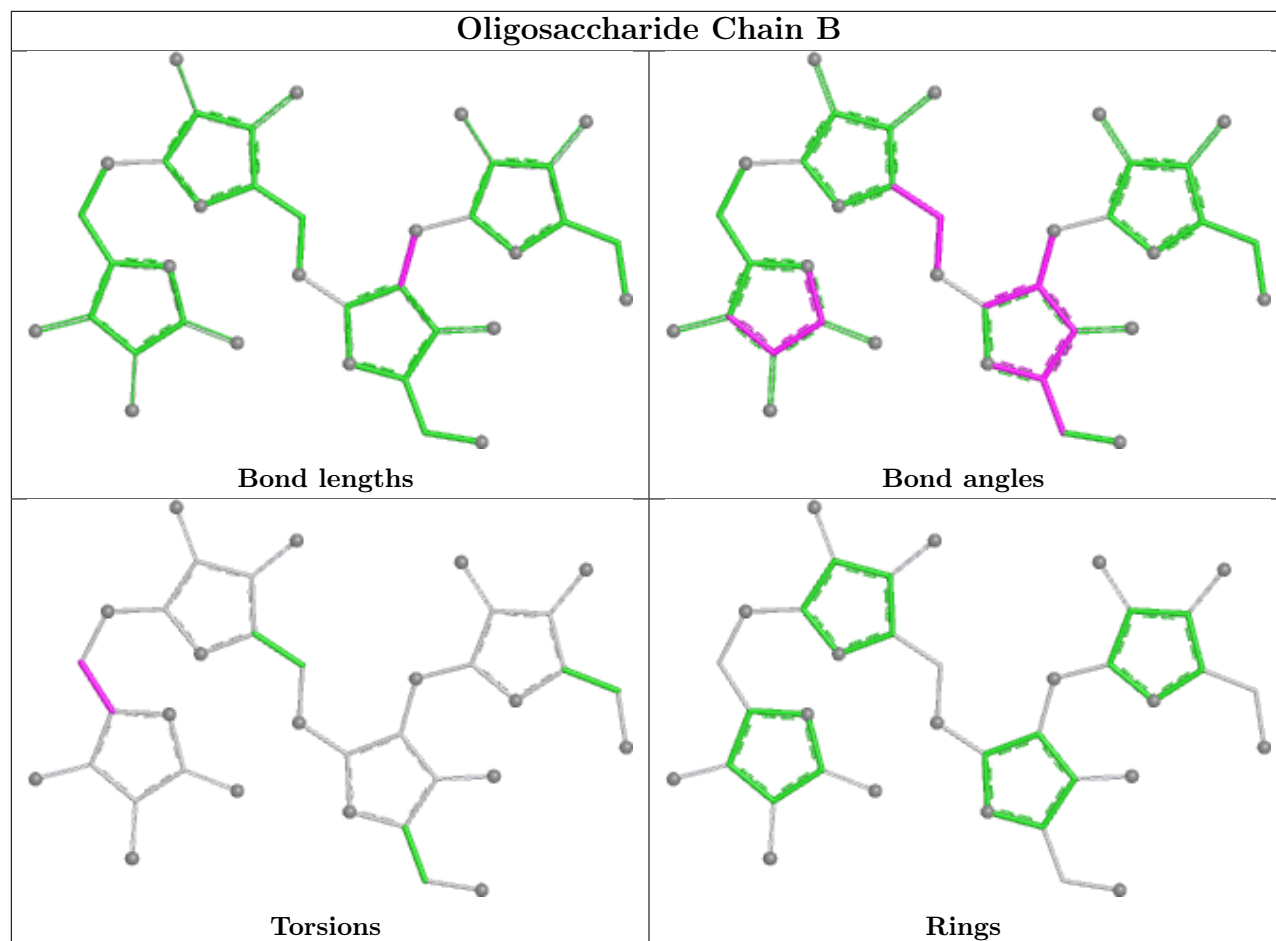
There are no ring outliers.

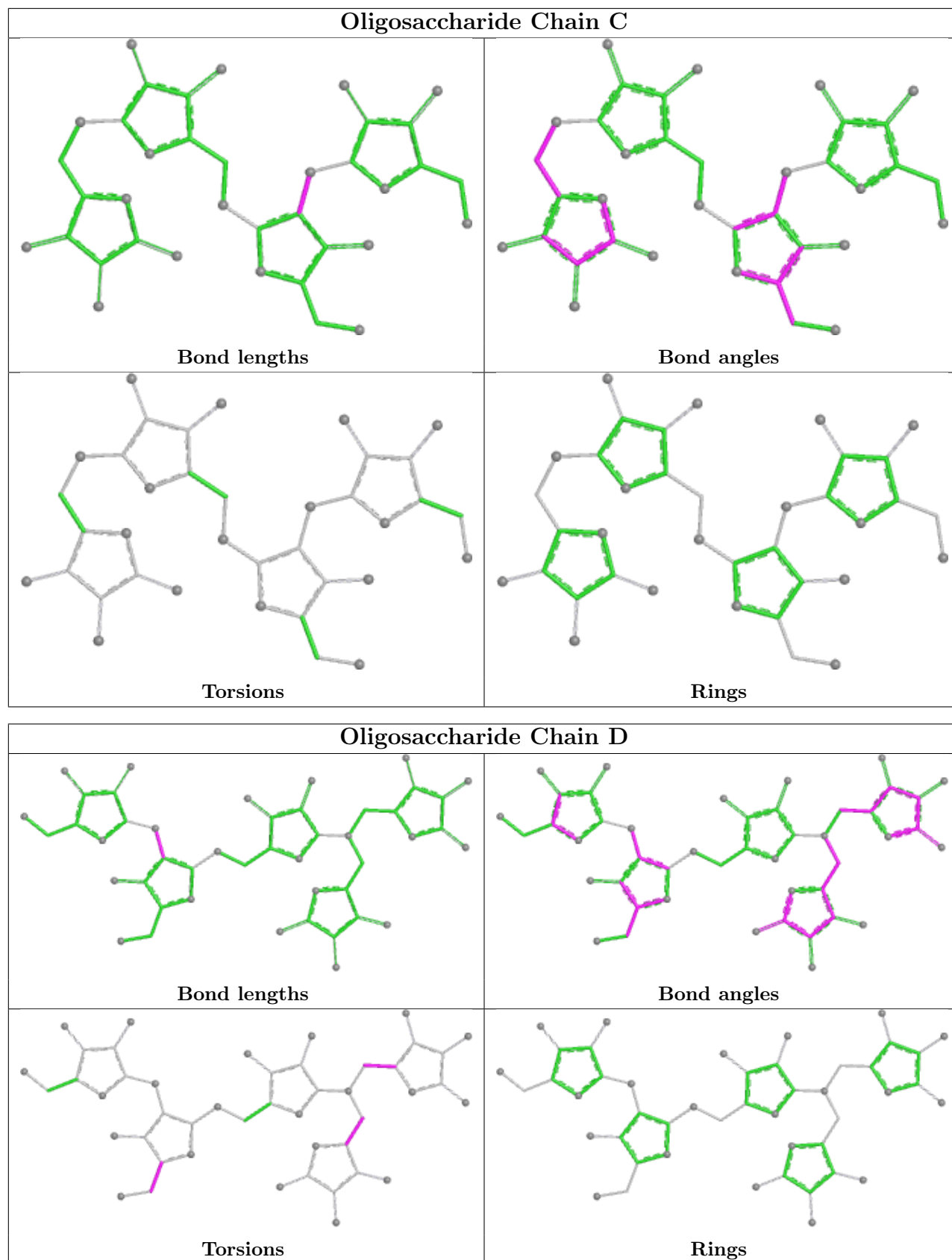
3 monomers are involved in 2 short contacts:

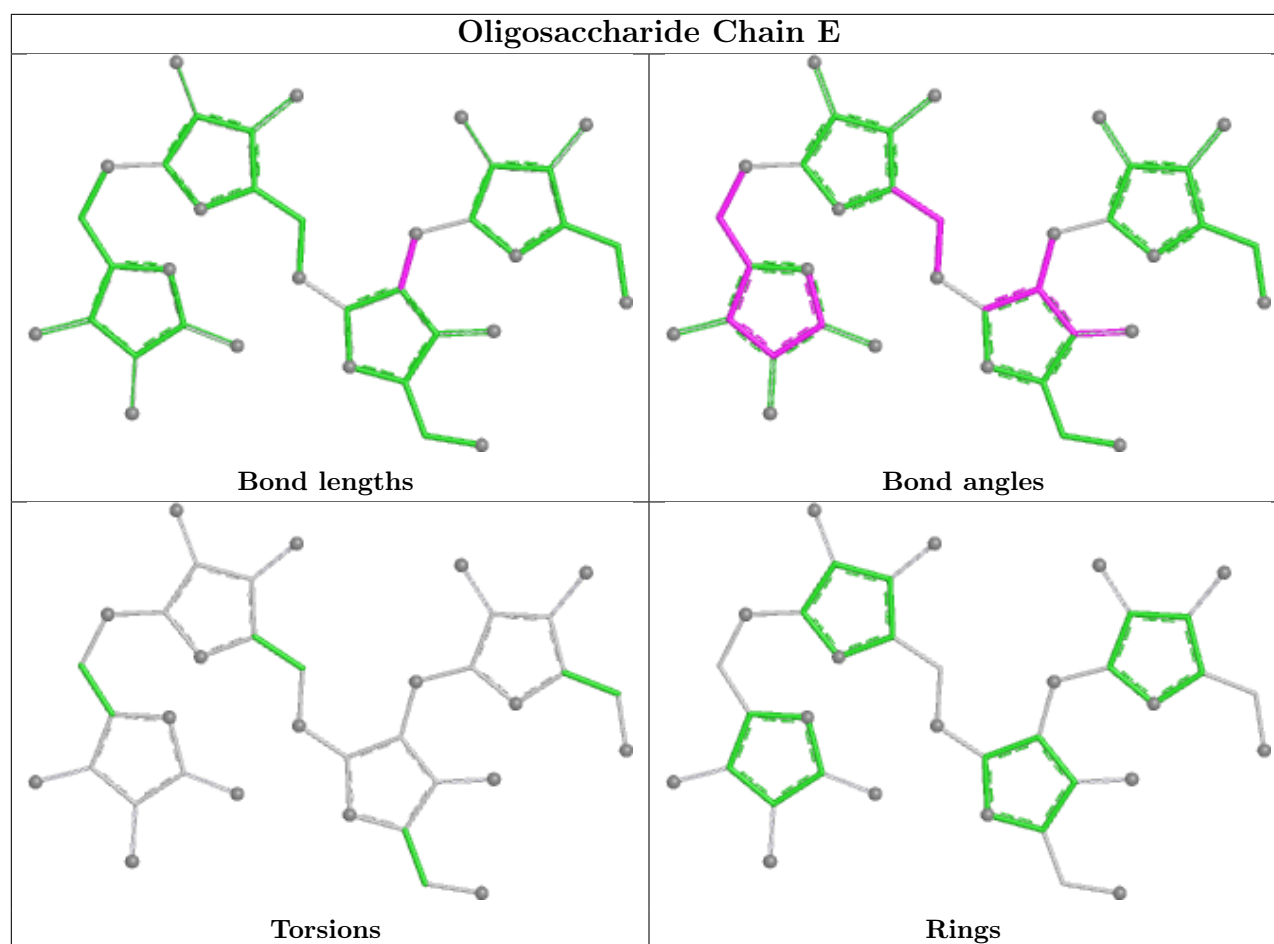
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1[A]	BXY	1	0
3	D	2	BXY	1	0
3	D	1[B]	BXY	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.









5.6 Ligand geometry [i](#)

15 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	EDO	H5	501	-	3,3,3	0.40	0	2,2,2	0.74	0
4	EDO	L3	302	-	3,3,3	0.52	0	2,2,2	0.21	0
4	EDO	H2	501	-	3,3,3	0.44	0	2,2,2	0.38	0
4	EDO	H4	501	-	3,3,3	0.47	0	2,2,2	0.38	0
4	EDO	L	301	-	3,3,3	0.38	0	2,2,2	0.66	0
4	EDO	H	501	-	3,3,3	0.38	0	2,2,2	0.57	0
4	EDO	H3	501	-	3,3,3	0.43	0	2,2,2	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	CIT	L4	301	-	12,12,12	1.05	0	17,17,17	1.68	3 (17%)
4	EDO	L3	301	-	3,3,3	0.43	0	2,2,2	0.43	0
4	EDO	H4	502	-	3,3,3	0.45	0	2,2,2	0.50	0
4	EDO	H	502[B]	-	3,3,3	0.47	0	2,2,2	0.31	0
4	EDO	H3	502	-	3,3,3	0.45	0	2,2,2	0.37	0
4	EDO	H	502[A]	-	3,3,3	0.48	0	2,2,2	0.27	0
4	EDO	L4	302	-	3,3,3	0.39	0	2,2,2	0.52	0
4	EDO	H2	502	-	3,3,3	0.48	0	2,2,2	0.27	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	H5	501	-	-	0/1/1/1	-
4	EDO	L3	302	-	-	1/1/1/1	-
4	EDO	H2	501	-	-	1/1/1/1	-
4	EDO	H4	501	-	-	1/1/1/1	-
4	EDO	L	301	-	-	1/1/1/1	-
4	EDO	H	501	-	-	1/1/1/1	-
4	EDO	H3	501	-	-	1/1/1/1	-
5	CIT	L4	301	-	-	4/16/16/16	-
4	EDO	L3	301	-	-	1/1/1/1	-
4	EDO	H4	502	-	-	1/1/1/1	-
4	EDO	H	502[B]	-	-	1/1/1/1	-
4	EDO	H3	502	-	-	1/1/1/1	-
4	EDO	H	502[A]	-	-	0/1/1/1	-
4	EDO	L4	302	-	-	1/1/1/1	-
4	EDO	H2	502	-	-	1/1/1/1	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L4	301	CIT	O6-C6-C3	4.61	121.99	113.14
5	L4	301	CIT	C2-C3-C6	2.09	114.67	110.03
5	L4	301	CIT	O4-C5-O3	-2.09	117.97	123.33

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L4	301	CIT	C1-C2-C3-O7
5	L4	301	CIT	C1-C2-C3-C4
5	L4	301	CIT	C1-C2-C3-C6
4	H3	502	EDO	O1-C1-C2-O2
4	L3	301	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L3	302	EDO	1	0
5	L4	301	CIT	1	0
4	H4	502	EDO	1	0
4	H2	502	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	H	216/228 (94%)	-0.53	1 (0%) 87 88	15, 35, 68, 106	3 (1%)
1	H2	217/228 (95%)	-0.35	2 (0%) 81 82	29, 42, 82, 103	2 (0%)
1	H3	215/228 (94%)	0.29	13 (6%) 27 24	29, 55, 122, 150	0
1	H4	217/228 (95%)	-0.45	3 (1%) 73 75	18, 37, 74, 104	1 (0%)
1	H5	217/228 (95%)	0.19	17 (7%) 19 16	24, 43, 111, 149	0
2	L	213/213 (100%)	-0.58	1 (0%) 87 88	20, 33, 63, 108	1 (0%)
2	L2	213/213 (100%)	-0.37	1 (0%) 87 88	22, 43, 70, 88	2 (0%)
2	L3	213/213 (100%)	-0.04	4 (1%) 66 67	16, 43, 103, 126	2 (0%)
2	L4	212/213 (99%)	-0.39	1 (0%) 87 88	20, 38, 81, 96	1 (0%)
2	L5	213/213 (100%)	-0.04	3 (1%) 73 75	28, 48, 96, 117	0
All	All	2146/2205 (97%)	-0.23	46 (2%) 63 65	15, 42, 96, 150	12 (0%)

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L2	213	CYS	5.7
2	L3	213	CYS	5.3
1	H3	212	ASN	4.4
2	L	213	CYS	4.4
1	H3	135	SER	3.9

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

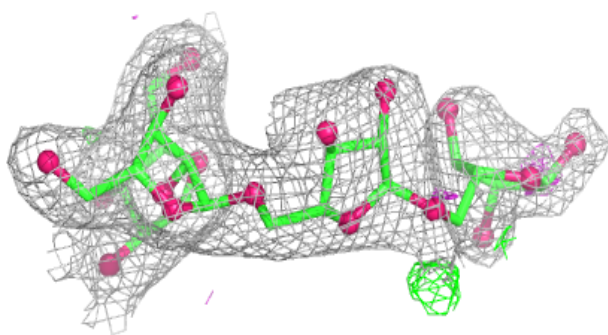
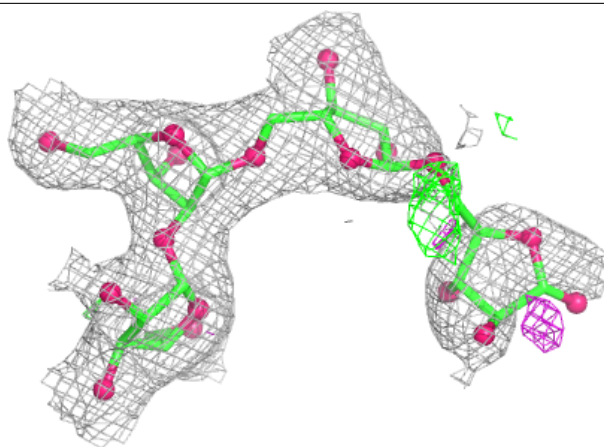
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BXY	A	1	10/10	-	-	91,98,104,104	0
3	BXY	A	2	9/10	-	-	30,45,63,71	0
3	BXY	A	3	9/10	-	-	25,28,29,30	0
3	BXX	A	4	9/10	-	-	23,25,32,32	0
3	BXY	B	1	10/10	-	-	91,102,109,110	0
3	BXY	B	2	9/10	-	-	42,53,65,72	0
3	BXY	B	3	9/10	-	-	30,31,34,35	0
3	BXX	B	4	9/10	-	-	28,32,35,37	0
3	BXY	C	1	10/10	-	-	82,101,106,107	0
3	BXY	C	2	9/10	-	-	40,59,69,77	0
3	BXY	C	3	9/10	-	-	31,37,38,38	0
3	BXX	C	4	9/10	-	-	29,36,49,49	0
3	BXY	D	1[A]	10/10	-	-	55,61,66,68	9
3	BXY	D	1[B]	10/10	-	-	46,60,66,68	9
3	BXY	D	2	9/10	-	-	29,44,55,58	0
3	BXY	D	3	9/10	-	-	26,27,29,36	0
3	BXX	D	4	9/10	-	-	26,27,33,34	0
3	BXY	E	1	10/10	-	-	79,101,107,111	0
3	BXY	E	2	9/10	-	-	33,47,64,65	0
3	BXY	E	3	9/10	-	-	26,29,33,37	0
3	BXX	E	4	9/10	-	-	20,26,28,31	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

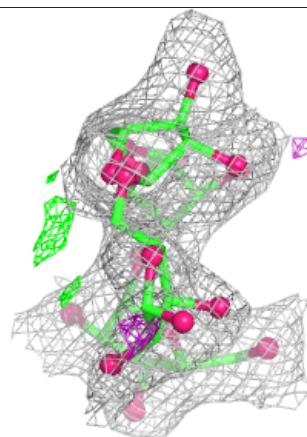
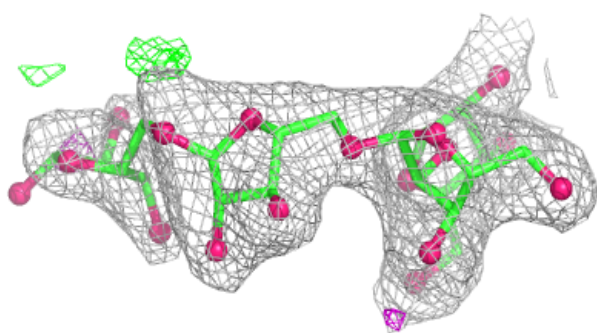
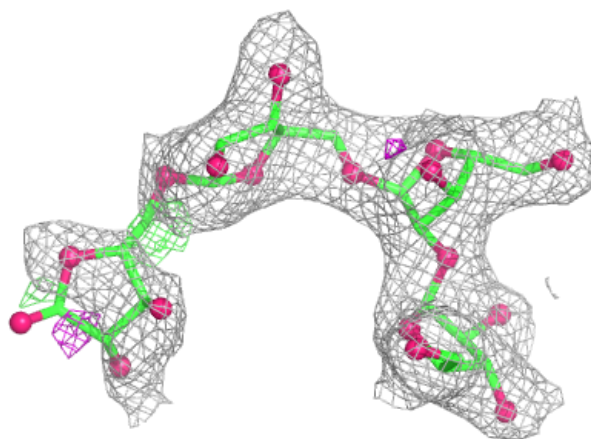
Electron density around Chain A:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



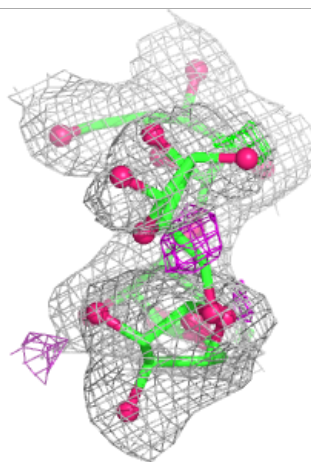
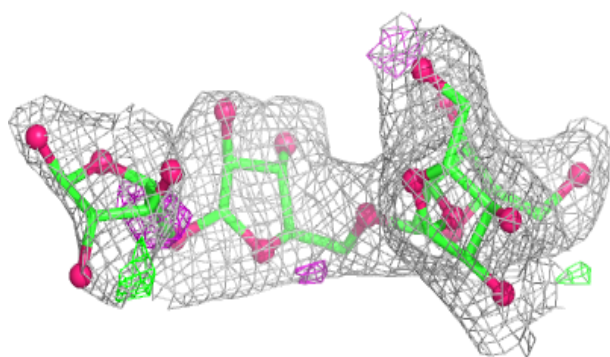
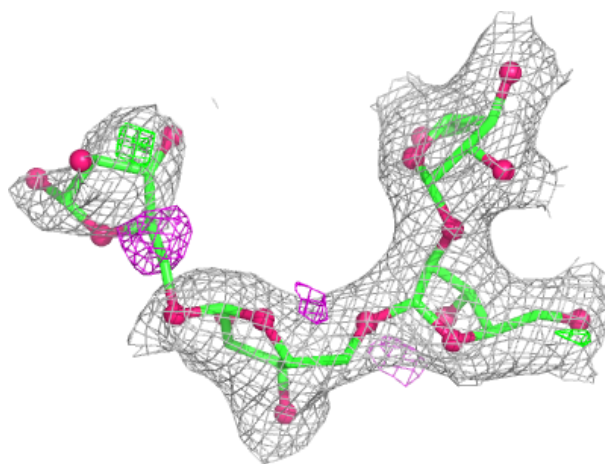
Electron density around Chain B:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



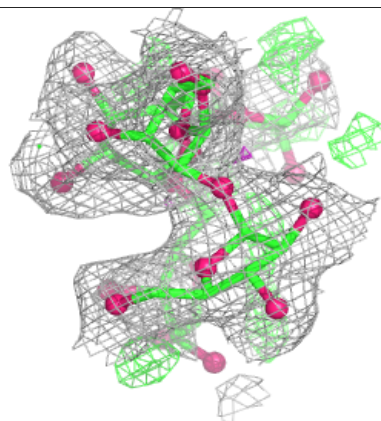
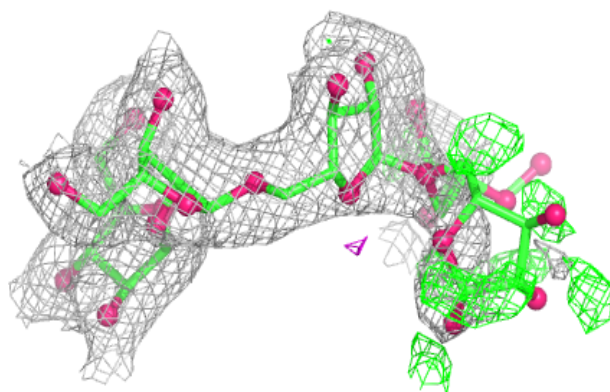
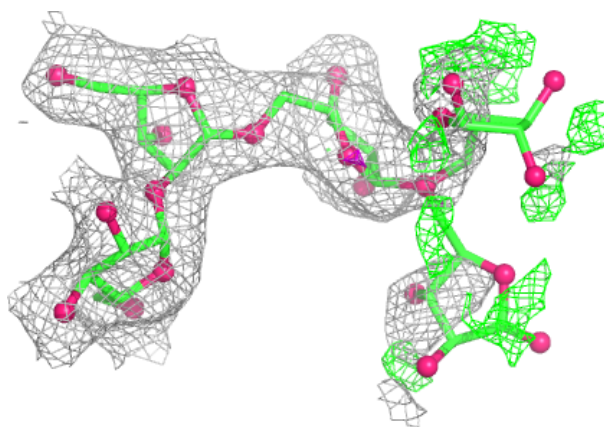
Electron density around Chain C:

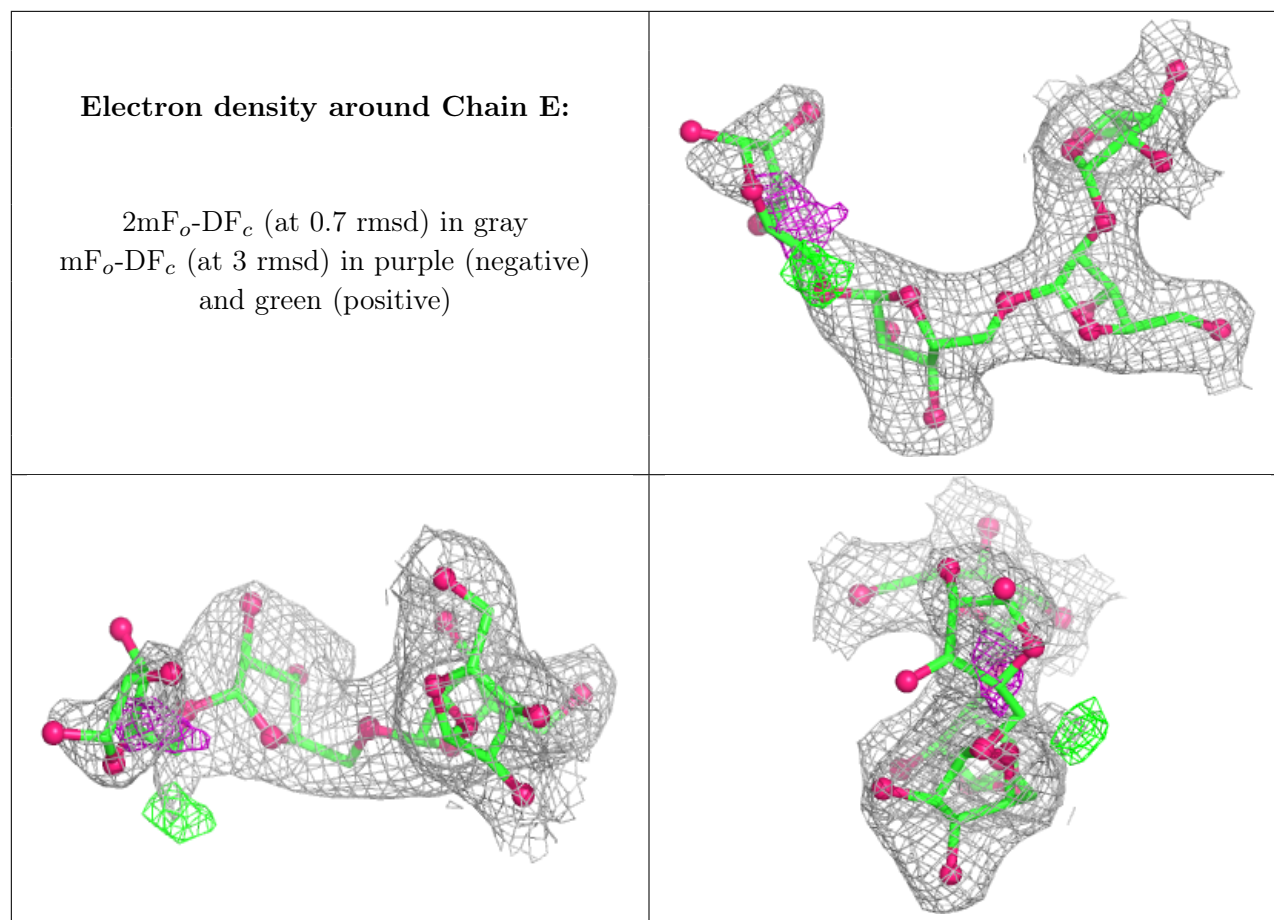
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain D:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	L3	301	4/4	0.52	0.25	61,67,68,69	0
4	EDO	H3	502	4/4	0.57	0.27	74,77,79,80	0
4	EDO	L4	302	4/4	0.61	0.18	79,80,82,86	0
4	EDO	H	502[B]	4/4	0.74	0.30	61,65,67,68	4
4	EDO	H	502[A]	4/4	0.74	0.30	59,64,67,67	4
4	EDO	L3	302	4/4	0.78	0.23	42,59,68,68	0
4	EDO	H4	502	4/4	0.84	0.19	63,64,71,80	0
5	CIT	L4	301	13/13	0.84	0.17	52,87,94,96	0
4	EDO	H5	501	4/4	0.88	0.15	58,62,64,65	0
4	EDO	H2	502	4/4	0.88	0.20	58,59,66,66	0
4	EDO	H3	501	4/4	0.90	0.11	58,59,63,63	0
4	EDO	H4	501	4/4	0.92	0.12	47,54,57,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	H	501	4/4	0.93	0.10	40,47,47,53	0
4	EDO	L	301	4/4	0.94	0.12	25,27,28,39	0
4	EDO	H2	501	4/4	0.94	0.09	43,53,59,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.